Solution Methods for Nonlinear Reaction-Diffusion Equations

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ABSTRACT: We seek to improve on traditional methods for the numerical simulation of reaction-diffusion equations by employing two-grid and operator splitting techniques. Two-grid methods and operator splitting methods can be used to help reduce computational cost and provide accurate, stable simulations.

Two-Grid Methods

First motivated by [3], two-grid methods provide a more efficient solution process for nonlinear partial differential equations on a mesh of size h. The method consists of two steps: first solving the original nonlinear problem on a much coarser grid of size H, then solving a linearized version of the problem on the original fine mesh. The coarse-grid solution will capture the nonlinear behavior of the problem, and the fine grid solve will refine the solution on a precise scale, resulting in a faster overall solution process. The theoretical application of this method to (1) was presented in [1].

Implementation

To incorporate the two-grid method into a time integration scheme, at each time step we use the following algorithm:

- On the coarse grid, find u_H that satisfies

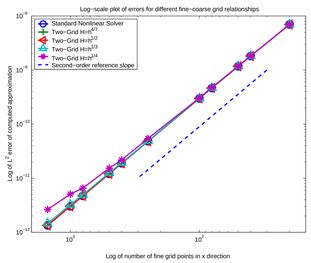
$$\frac{\partial u_H}{\partial t} = \nabla \cdot (K(u_H)\nabla u_H) + r(\mathbf{x}, u_H)$$

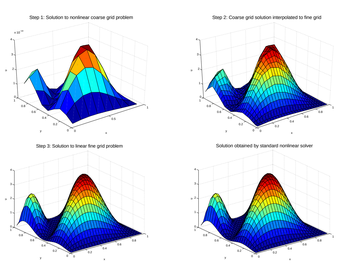
- Interpoate u_H to the fine grid
- On the fine grid, find u_h that satisfies

$$\frac{\partial u_h}{\partial t} = \nabla \cdot [K_u(u_H)\nabla u_H(u_h - u_H) + K(u_H)\nabla u_h] + r_u(\mathbf{x}, u_H)(u_h - u_H)$$

Our Work

We have implemented the two-grid method for (1) within the context of a second-order backward differentiation formula implicit time-stepping scheme. **The size of the nonlinear problem is significantly reduced, and the method has shown to preserve the order of accuracy of the standard nonlinear solver approach.** We are focusing our investigations on the relationship between the coarse and fine grid sizes as well as alternate formulations of the two-grid algorithm, which include additional fine grid linear corrections or possibly higher-order coarse grid linear corrections.





Introduction

The general model for a reaction-diffusion system is given by

$$\frac{\partial u}{\partial t} = \nabla \cdot (K(u)\nabla u) + r(\mathbf{x}, u) \quad \text{in } \Omega \times (0, T). \tag{1}$$

with boundary conditions

$$u = g_D \quad \text{on } \Gamma_D \quad \text{and} \quad -K(u)\nabla u = g_N \quad \text{on } \Gamma_N$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$ and initial condition

$$u(\mathbf{x}, 0) = \mathbf{u}^0 \quad \text{in } \Omega.$$

Applications of this model include energy transport in stellar and laser fusion, porous media flow, biogeochemical phenomena, as well as many others.

Solution Approach

Using (1) and the lowest-order Raviart-Thomas-Nedélec spaces on rectangular boxes and particular choices of quadrature rules, we arrive at a cell-centered finite difference (CCFD) discretization of u_t. This discretization is second-order accurate in space ($O(h^2)$). We then must solve the system of ordinary differential equations

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}). \tag{2}$$

To integrate the solution with respect to time, we use implicit backward differentiation formulas (BDF). Thus, in order to progress from time t_n to time t_{n+1}, we must solve a large system of nonlinear equations. Two-Grid methods and Operator Splitting methods give us different ways to tackle problem (2).

Conclusions and Future Work

- Two-grid methods have shown numerically to have the same accuracy as the standard approach with less computational time spent in nonlinear solver routines.
- Optimimzed two-grid code should result in an overall faster solution process.
- Alternate formulations of the two-grid algorithm are being tested to determine if they provide even better performance, as well as investigations into the relationship between the fine and coarse grid sizes.
- Operator splitting methods show promise in being able to solve nonlinear reaction-diffusion problems efficiently.
- Appropriate implicit schemes will be constructed to meet the specifications for different splitting methods without the loss of accuracy.

References

[1] C. N. Dawson, M. F. Wheeler, and C. S. Woodward. A two-grid finite difference scheme for nonlinear parabolic equations. *SIAM Journal on Numerical Analysis*, 35(2):435–452, April 1998.

[2] G. Strang. On the construction and comparison of different schemes. *SIAM Journal on Numerical Analysis*, 5(3):506–517, 1968.

[3] J. Xu. Two-grid discretization techniques for linear and nonlinear PDEs. *SIAM Journal on Numerical Analysis*, 33(5):1759–1777, October 1996.

Operator Splitting Methods

Operator splitting or fractional step methods seek to simplify the nonlinear system formed by (2) by separating the reaction and diffusion operators in (1):

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}) = \mathbf{f}_{\mathcal{D}}(t, \mathbf{u}) + \mathbf{f}_{\mathcal{R}}(t, \mathbf{u}) \tag{3}$$

Each operator is then integrated in time individually (with temporal integrators designed for each) and the result from each fractional step is used as initial data for the subsequent fractional step. In operator notation, with $\mathcal{D}$ representing the diffusion operator and $\mathcal{R}$ representing the reaction operator, to find $\mathbf{u}_{n+1}$ given $\mathbf{u}_n$ and $t_{n+1} = t_n + \Delta t$, a simple first-order splitting scheme can be written as

$$\mathbf{u}_{n+1} = \mathcal{D}_{\Delta t}\mathcal{R}_{\Delta t}\mathbf{u}_n.$$

Example: Strang Splitting

Strang splitting [2] is a second-order accurate in time splitting method that, over one external time step, applies one operator for a half time step, then the other operator for a full time step, then finally the first operator for the remaining half step. If we apply the reaction operator first, Strang splitting (RDR) applied to (3) over one time step consists of solving:

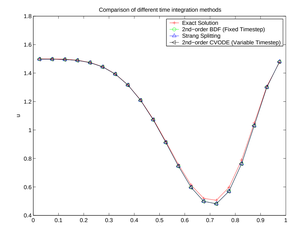
$$\frac{d\mathbf{u}^*}{dt} = \mathbf{f}_{\mathcal{R}}(t, \mathbf{u}^*) \quad \text{on } [0, \Delta t/2], \quad \mathbf{u}^*(0) = \mathbf{u}(t_n)$$

$$\frac{d\mathbf{u}^{**}}{dt} = \mathbf{f}_{\mathcal{D}}(t, \mathbf{u}^{**}) \quad \text{on } [0, \Delta t], \quad \mathbf{u}^{**}(0) = \mathbf{u}^*(\Delta t/2)$$

$$\frac{d\mathbf{u}^{***}}{dt} = \mathbf{f}_{\mathcal{R}}(t, \mathbf{u}^{***}) \quad \text{on } [\Delta t/2, \Delta t], \quad \mathbf{u}^{***}(0) = \mathbf{u}^{**}(\Delta t)$$

Our Work

We are implementing various operator splitting schemes to advance the solution of (3) at each timestep for the problem (1). Unlike most previous applications of operator splitting methods that use combinations of implicit and explicit methods, we are interested in using fully implicit methods (such as specially-constructed backward differentiation formulas) for use in each fractional step. Preliminary numerical results show that for sample problems the splitting methods are very close in accuracy to CVODE, an implicit variable time step stiff ODE solver developed at LLNL, as well as the standard BDF method.



Goal:
To evaluate the relative accuracy and cost benefit of operator splitting and fully implicit time integration schemes.

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